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Thesis Title: Stereoselective Homogeneous Catalysis

Abstract

Stereoselective homogeneous catalysis is present in many products used on a daily basis. Stereoselective hydroformylation presents a one-step means of converting simple olefins into pharmaceutical intermediates. Despite this, little is known about the occurrences that happen inside the autoclave. *In situ* FTIR spectroscopy coupled with chemometrics and chiral GC, were carried out in this study to address this issue as it applies to stereoselective hydroformylation of styrene by $\text{Rh}_4(\text{CO})_{12}$ and (S)-BINAP. Turnover frequencies were evaluated on the basis of the dominant organometallic species present, and the effects of all variables were explored.

Generation of this species with the standard metal precursor is an important issue. However, little is known about the chemistry between diphosphines and $\text{Rh}_4(\text{CO})_{12}$. NMR studies were undertaken to elucidate the initial steps of attack of (S)-BINAP, as well as several bis(diphenylphosphino)alkanes, on the $\text{Rh}_4(\text{CO})_{12}$ cluster.

Keywords: Stereoselective hydroformylation homogenous catalysis pharmaceuticals *in-situ*